ReaxysFile™

Subject Coverage

Extensive chemistry content:

- All types organic and inorganic substances, including alloys, coordination compounds, minerals, mixtures, polymers, salts
- Properties and Reaction Data (from following list, if available)

- Chemical data
- Electrochemical behaviour
- Electrical and magnetic properties
- Identification of substance
- Materials composition data
- Multi-component systems
- Optical properties
- Patent specific data
- Pharmacological and ecological data
- Physical and mechanical properties
- Reactions/preparations
- Safety data
- Spectroscopic data
- State of aggregation
- Structure and energy parameter
- Thermodynamic properties
- Transport phenomena

File Type

Structure

Features

Alerts (SDIs)	Not available		
CAS Registry Number® Identifiers	☑	SLART	☐
Keep & Share	☐	Structures	☑

Record Content

- Substance Identification Data (chemical name, molecular formula, etc.)
- Properties (if available)
- Reactions (if available)
- Bibliographic/patent data

File Size

19,404,345 substance records

Coverage

1771-2011

Updates

Static File

Language

English

Database Producer

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CH-2000, Neuchâtel
Switzerland

Sources

- Appr. 450 chemistry core journals plus periodicals related to Chemistry
- Patents from selected authorities

User Aids	• Building and Searching Structures on STN • Online Helps (HELP DIRECTORY lists all help messages available) • STNGUIDE
Cluster	• CASRNS • NUMERIC • STRUCTURE STN Database Cluster information: https://www.cas.org/support/training/stn/database-clusters

FACTUAL SEARCHING

Search and Display Field Codes

There are no fields that allow left truncation.

Substance Identifying Information

Search Field Name	Search Code	Search Examples	Display Codes
Basic Index (contains single 'words' from ADSM.PA **(1),** ADSM.PAAN, ASSM.PA **(1)**, ASSM.PAAN, AUN, AZE.PA **(1),** AZE.PAAN, BPR, AN, BSPM.PA **(1)**, BSPM.PAAN, CDER **(1)**, CDER.AN, CN **(1)**, COMPAN, COMPN **(1)**, CPEM.PA **(1)**, CPEM.PAAN, EDM.PA **(1)**,EDM.PAAN, ENEM.PA **(1)**, ENEM.PAAN, FAN, FMF, HHDG.AN, HHDG.CN **(1)**, INP **(1)**, LLSM.PA **(1),** LLSM.PAAN, LSSM.PA **(1)**, LSSM.PAAN, LVSM.PA **(1)**, LVSM.PAAN, MECM.PA **(1)**, MECM.PAAN, MF, ODM.PA **(1)**, ODM.PAAN, POT.PAN, POT.PRO **(1)**, RN, RSTR.PA **(1)**, RSTR.PAAN, TRAM.PA **(1)**, TRAM.PAAN, SOLM.PA **(1)**, SOLM.PAAN, XREF.CN **(1)**, and all 'Code.KW' fields)	None or /BI	S ETHYL	ADSM, ASSM, AUN, AZE, BPR, AN, BSPM, CDER, CN, COMPAN, COMPN, CPEM, EDM, ENEM, FAN, FMF, HHDG, INP, LLSM, LSSM, LVSM, MECH, MF, ODM, POT, RSTR.TRAM, RN, STR, SOLM, XREF, CODE **(2)**
Basic Index Pharmacological and Ecological Data (contains all fields from PED data: BIO, BIOD, COEV, ECDH, ECDP, ECTD, ECTOX, EOD, EXCA, PHARM, USC)	/BIPED	S (AQUA? TOX?)/BIPED	BIO, BIOD, BPSM, COEV, ECDH, ECDP, ECTD, ECTOX, EOD, EXCA, PHARM, USC
Accession Number	/AN	S 1915876/AN	AN
All Keywords	/AKW	S CHEMICAL SHIFTS/AKW	all display codes for Code.KW fields
Alternate InChi Key	/AINCHI	S KWEZFXJCZZEGTG-JGRHXJNXBK/AINCHI	AINCHI
Basic Preferred Registry Number	/BPR	S 106-24-1/BPR	BPR
CAS Registry Number	/RN	S 100-03-8/RN	RN
Chemical Name **(1)**	/CN	S CHOLESTEROL/CN	CN, AUN **(4)**
Chemical Name Segment **(1)**	/CNS	S CHOLESTERYL/CNS	CN
Composition: Comp. AN **(3)**	/COMPAN	S 5811/COMPAN	COMPAN
Composition: Comp. Name	/COMPN	S POLYVINYLPYRROLIDONE /COMPN	COMPN
Compound Type	/CTYPE	S ETHYLENE/CNS AND POLYMER?/CTYPE	CTYPE
Data Entry Date	/DED	S 1990?/DED	DED
Data Update Date	/DUPD	S 2010/01/1124/DUPD	DUPD
Element Count (specific) **(3)**	/ELEMENT SYMBOL	S 5/CL	MF
Element Ratio	/ELR.XX	S 2/ELR.HC AND 0.5/ELR.OC	MF
Element Symbol	/ELS	S O/ELS AND SE/ELS	MF

Search and Display Field Codes
Substance Identifying Information (cont'd)

Search Field Name	Search Code	Search Examples	Display Codes
Field Availability **(5)**	/FA	S ISOELECTRIC POINT/FA	FA **(6)**
Field Not Availability	/FNA	S ALCOHOL/CNS AND BP/FNA	not displayed
Formula Weight **(3)**	/FW (or /MW)	S 3000<FW	FW
Fragment AN **(3)**	/FAN	S 1073/FAN	FAN
Fragment Molecular Formula	/FMF	S C6H12O6/FMF	FMF
InChi Key	/INCHI	S KWEZFXJCZZEGTG-JGRHXJNXSA-N/INCHI	INCHI
Linearized Structure Formula	/LSF	S "CH2O(1+)"/LSF	LSF
Molecular Formula	/MF	S C4H9N5.H3O4P/MF	MF
Number of Atoms **(3)**	/ATC	S 34-36/ATC	MF
Number of Elements **(3)**	/ELC	S 5/C AND 5/ELC	FMF, MF
Number of Fragments **(3)**	/NF	S 3/NF	MF
Patent Specific Data	/PSD	S PSD/FA	PSD
Periodic Group	/PG	S (A3 AND A6)/PG	not displayed
Substance Label	/LB	S LINE16/LB	LB
STN Update Date **(3)**	/UP	S L1 AND 20020701-20020731/UP	not displayed
Structure Image		STR 1209246	

(1) Input partly in German.
(2) All codes with keywords.
(3) Numeric search field that may be searched using numeric operators or ranges.
(4) The CN display field contains, if available, the Chemical Name (CN) and the AUTONOM Name (AUN).
(5) Searching for all information available for each display field.
(6) DISPLAY FA shows all display field codes available for a record.

Search and Display Field Codes
Bibliographic Information

Search Field Name	Search Code	Search Examples	Display Codes
Author **(1)**	/AU	S SHARPLESS?/AU	
Citation (unresolved	/URES	S PERKIN?/URES	
Document Type **(1)**	/DT	S PATENT/DT	not displayed
International Standard (Document) Number (CODEN)	/ISN	S JACSAT/ISN	
Inventor	/IN	S CRAMER/IN	IN
Journal Title **(1)**	/JT	S TETRAHEDRON/JT	
Journal/Review without CODEN	/JTW	S "JOURNAL OF THE SOCIETY OF DYERS AND COLOURISTS"/JTW	
Language	/LA	S JAPANESE/LA	not displayed
Patent Assignee **(1)**	/PA	S BASF/PA	
Patent Number **(1)**	/PN	S DE 670683/PN	
Publication Year **(1,2)**	/PY	S JACSAT/ISN AND 2009/PY	

(1) To restrict search to bibliographic information in substance documents, append .SUB to the search field code, e.g., /JT.SUB. To restrict search to reaction data, append .RX to the search field code, e.g., /AU.RX.
(2) Numeric search field that may be searched using numeric operators or ranges.

Super Search Fields [1)]

Search Field Name	Search Code	Fields Searched	Search Examples	Display Codes
All Journal Titles (incl. titles in JT, JTW, and URES)	/AJT	/JT, /JTW, /URES	S IMMUNOCHEMISTRY/AJT	
All Record Numbers	/AAN	/AN, /COMPAN, /FAN, /AZE.AN, /CPEM.PAAN /ENEM.PAAN /EDM.PAAN, /BSPM.PAAN /ADSM.PAAN /ASSM.PAAN /LVSM.PAAN /LLSM.PAAN /LSSM.PAAN /MECM.PAAN /TRAM.PAAN /ODM.PAAN, /RSTR.PAAN /HHDG.AN, /POT.PAN, /CDER.AN, /PHARM.AN, /ECTOX.AN, /BIOD.AN, /ECDH.AN, /ECDP.AN		ADSM, ASSM, AZE, BIOD, AN, BSPM, CDER, COMPAN, CPEM, ECDH,ECDP, ECTOX, EDM, ENEM, FAN, HHDG, LLSM, LSSM, LVSM, MECM, ODM, PHARM, POT, RSTR, SOLM, TRAM
Reaction	/RX	/RX.RCT, /RX.RGT, /RX.PRO, /RX.SUBJ, /RX.SOL, /RX.CAT, /RX.TYP, /RX.PRT, /RX.SRCT	S (ACETIC ACID)/RX	RX

(1) Enter a super search code to execute a search in one or more fields that may contain the desired information. Super search fields facilitate crossfile and multifile searching. EXPAND may not be used with super search fields. Use EXPAND with the individual field codes instead.

Search and Display Field Codes

Chemical Data

Search Field Name	Search Code	Search Examples	Display Codes
Chemical Derivative			
Derivative **(1)**	/CDER	S 8116437/AN AND HYDRAZONE/CDER	CDER
Derivative AN **(2)**	/CDER.AN	S 5845535/CDER.AN	CDER
Derivative Comment **(1)**	/CDER.COM	S BENZIMIDAZOLE/CDER.COM	CDER
Derivative Melting Point (2)	/CDER.MP	S 50/CDER.MP	CDER
Isolation from Natural Product (1)	/INP	S LEAVES/INP	INP
Comment **(1)**	/INP.COM	S DEXTROROTATORY/INP.COM	INP
Purification (method) (1)	/PUR	S ALCOHOL/CNS AND ACETYLATION/PUR	PUR
Related Structure (1)	/RSTR	S CONSTITUTION/RSTR	RSTR
Comment **(1)**	/RSTR.COM	S HANDBOOK/RSTR.COM	RSTR
Referenced Compound **(1)**	/RSTR.PA	S OESTRADIOLDIMETHYLETHER/RSTR.PA	RSTR
Referenced AN **(2)**	/RSTR.PAAN	S 1581/RSTR.PAAN	RSTR

Chemical Data (cont'd)

Search Field Name	Search Code	Search Examples	Display Codes
Crossfile Reference			
Data Type	/XREF.DTP	S 6279685/AN AND IR/XREF.DTP	XREF
External Access ID	/XREF.ID	S ALDRICH/XREF.SO AND 250619/XREF.ID	XREF
Name **(1)**	/XREF.CN	S N-BENZOYL-4-PIPERIDONE/XREF.CN	XREF
Other Source	/XREF.SO (or /OS)	S MERCK INDEX/OS	XREF

(1) Input partly in German.
(2) Numeric search field that may be searched using numeric operators or ranges.

Reaction Data

Search Field Name	Default Units	Fields Searched	Search Examples	Display Codes
Reaction Basic Index (contains single words from RX.CAT, RX.CL, RX.COM, RX.COND, RX.PAN, RX.PRO, RX.RAN, RX.RCT, RX.RGT, RX.SOL, RX.SRAN, RX.SRCT, RX.SUBJ,RX.TYP)	-	/BIRX	S CONDENSATION/BIRX	RX
All AN Reaction **(1,2)**	-	/RX.AAN	S 50000/RX.AAN	RX
Catalyst AN **(2)**		/RX.CAAN	S 1073/RX.CAAN	RX
Catalyst **(3)**	-	/RX.CAT	S SNBR2/RX.CAT	RX
Reaction Classification **(3)**	-	/RX.CL	S (CHEMICAL(W)BEHAVIOUR)/RX.CL	RX
Other Conditions **(3,4)**	-	/RX.COND	S ICEWATER/RX.COND	RX
Reaction ID **(2)**	-	/RX.ID	S 5418675/RX.ID	RX
Multi Step Details		/RX.MTEXT	S 25007/RX.MTEXT	RX
No. of Reaction Details **(2)**	-	/RX.NVAR	S 2/RX.NVAR	RX
Pressure **(2,3)**	Torr	/RX.P	S 1-25/RX.P	RX
Product AN **(2)**	-	/RX.PAN	S 4885619/RX.PAN	RX
pH Value **(2,3)**	-	/RX.PH	S RX.PH<1	RX
Product AN (detail)		/RX.PRAN	S 925/RX.PRAN	RX
Product **(4)**	-	/RX.PRO	S "CHLORPROMAZINE N+-GLUCURONIDE CHLORIDE"/RX.PRO	RX
Prototype Reaction **(3)**	-	/RX.PRT	S CATALYST?/RX.PRT	RX
Reactant AN **(2)**	-	/RX.RAN	S 5026/RX.RAN	RX
Reactant AN (from detail) **(2)**		/RX.RCAN	S 1073/RX.CAN	RX
Reactant **(4)**	-	/RX.RCT	S L-PROLINE/RX.RCT	RX
Reagent **(3,4)**	-	/RX.RGT	S ACETONE/RX.RGT	RX
Reaction Details Reaction ID **(3)**	-	/RX.RID	S 1000.2/RX.RID	RX
Number of Stages **(3)**	-	/RX.SNR	S 2/RX.SNR	RX
Solvent **(3)**	-	/RX.SOL	S CH2CL2/RX.SOL	RX
Stage Reactant AN **(2,3)**	-	/RX.SRAN	S 742586/RX.SRAN	RX
Stage Reactant **(3,4)**	-	/RX.SRCT	S MALONALDEHYDE/RX.SRCT	RX
Stage Number		/RX.STG	S 2/RX.STG	RX
Number of Steps		/RX.STP	S 2/RX.STP	RX
Subject Studied **(3)**	-	/RX.SUBJ	S KINETICS/RX.SUBJ	RX
Temperature **(2)**	Cel	/RX.T	S -100 - -10/RX.T	RX
Time **(3)**	-	/RX.TIM	S "2.0 HOUR(S)"/RX.TIM	RX
Reaction Type **(3)**	-	/RX.TYP	S POLYMERIZATION/RX.TYP	RX
Yield (optical)		/RX.YDO	S 10 PERCENT DE/RX.YDO	RX
Yield (numerical)		/RX.YDN	S 25.01/RX.YDN	RX
Yield Data **(3,5)**		/RX.YDT	S 2-10 PERCENT/RX.YDT	RX
Yield (Product)	-	/RX.YPRO	S METHACROLEIN/RX.YPRO	RX

Reaction Data (cont'd)

Search Field Name	Default Units	Fields Searched	Search Examples	Display Codes
Solvent AN **(2)**	-	/RX.SOLAN	S 1159/RX.SOLAN	RX
Record Type		/RX.RTYP	S FULL REACTION/RX.RTYP	RX
Number of References **(2)**		/RX.NUMREF	S 10/RX.NUMREF	RX
Example Label	-	/RX.LB	S FIGURE/RX.LB	RX
Example Title		/RX.TI	S RELEASE/RX.TI	RX
Fulltext of Reaction		/RX.TXT	S CONTROLLED/RX.TXT	RX
Location in Patent		/RX.LCN	S COLUMN/RX.LCN	RX
Reaction Structure Keyword		/RX.SKW	S MAPPED/RX.SKW	RX
Number of Bond Changes		/RX.NBC	Display only	RX
Preparation Reactants **(2)**		/RX.BLB	S 1004/RX.BLB	RX
Det. Reaction Reactant **(2)**		/RX.BLC	S 1033/RX.BLC	RX

(1) A search in /RX.ABAN includes the parameters: Reactant AN, Product AN and Stage Reactant AN.
(2) Numeric search field that may be searched using numeric operators or ranges.
(3) Reaction Detail: Included in the default display format QRD only when searched for a reaction detail.
(4) Input partly in German.
(5) Values given for yield in the /RX.YD and /RX.YDT are identical but the numeric yield field (/RX.YD) does not exist for all reactions.

Electric and Magnetic Properties

Search Field Name	Default Units	Fields Searched	Search Examples	Display Codes
Dielectric Constant (1)	none	/DIC	S 2-2.2/DIC	DIC
Comment **(2)**	-	/DIC.COM	S HEPTAN/DIC.COM	DIC
Frequency **(1)**	Hz	/DIC.F	S 50000/DIC.F	DIC
Temperature **(1)**	Cel	/DIC.T	S 20.5/DIC.T	DIC
Electrical Data	-			
Comment **(2)**	-	/ELE.COM	S PHENOL/ELE.COM	ELE
Critical Superconductivity Temperature (1)	Cel	/ELE.CRIT	S -201.16/ELE.CRIT	ELE
Conductivity (1)	S/cm	/ELE.ECVAL	S 4/ELE.ECVAL	ELE
Description	-	/ELE.KW	S PIEZOELECTRICITY/ELE.KW	ELE
Temperature (1)	Cel	/ELE.T	S 216.84/ELE.T	ELE
Magnetic Data	-			MAG
Comment **(2)**	-	/MAG.COM	S INFLUENCE/MAG.COM	MAG
Description	-	/MAG.KW	S SPIN/MAG.KW	MAG
Temperature (1)	Cel	/MAG.T	S 129/MAG.T	MAG
Moment (1)	A*cm**2	/MAG.MMOM	S 9.21/MAG.MMOM	MAG
Magnetic Susceptibility (1)	cm**3/mol*E6	/MSUS	S 0-410/MSUS	MSUS
Comment **(2)**	-	/MSUS.COM	S RANGE/MSUS.COM	MSUS
Temperature **(1)**	CEL	/MSUS.T	S 20-25/MSUS.T	
Static Dielectric Constant (1)	none	/DICS	S 2.3-2.301/DICS	DICS
Comment **(2)**	-	/DICS.COM	S POLARISATION/DICS.COM	DICS
Temperature **(1)**	Cel	/DICS.T	S DICS.T>20	DICS

(1) Numeric search field that may be searched using numeric operators or ranges.
(2) Input partly in German.

Electrochemical Behaviour and Data

Search Field Name	Default Units	Fields Searched	Search Examples	Display Codes
Dissociation Exponent (pK) (1)	**-**	/DE	S 1.5-1.55/DE	DE
Comment **(2)**	**-**	/DE.COM	S HANDBOOK/DE.COM	DE
Method	**-**	/DE.MET	S CONDUCTOMETRIC/DE.MET	DE
Solvent	**-**	/DE.SOL	S D2O/DE.SOL	DE
Temperature **(1)**	Cel	/DE.T	S DE.T>180	DE
Type	-	/DE.TYP	S THERMODYNAMIC/DE.TYP	DE
Electrochemical Behaviour				
Comment **(2)**	**-**	/ELCB.COM	S GAS/ELCB.COM	ELCB
Description	-	/ELCB.KW	S PROTON AFFINITY/ELCB.KW	ELCB
Isoelectric Point pH (1)	-	/IEP	S IEP>5.5	IEP
Comment **(2)**	-	/IEP.COM	S ACID/IEP.COM	IEP
Solvent	-	/IEP.SOL	S H2O/IEP.SOL	IEP
Electrochemical Characteristics	-			
Comment **(2)**	-	/POT.COM	S CYCLOVOLTAMMETRY/POT.COM	POT
Description	-	/POT.KW	S OXIDATION POTENTIAL/POT.KW	POT
pH-Value **(1)**	-	/POT.PH	S 1-7/POT.PH	POT
Product	-	/POT.PRO	S PHENYLENEDIAMINE/POT.PRO	POT
Product AN **(1)**	-	/POT.PAN	S 23241/POT.PAN	POT
Solvent	-	/POT.SOL	S METHANOL/POT.SOL	POT
Temperature **(1)**	Cel	/POT.T	S POT.T<-10	POT
Electrochemical Cell				
Electrochemical Cell	-	/ELCH.ECELL	S ACETATE/ELCH.ECELL	ELCH
Cell Potential(1)	c	/ELCH.POT	S 1/ELCH.POT	ELCH
Keyword	-	/ELCH.KW	S ELECTROLYSIS/ELCH.KW	ELCH
Comment	-	/ELCH.COM	S AMOUNT/ELCH.COM	ELCH
Electrolytic Conductivity				
Electrolytic Conductivity **(1)**	S*1/(cm*mol)	/ELYC.VAL	S 1/ELYC.VAL	ELYC
Equivalent Conductivity **(1)**	S*cm**2/val	/ELYC.EVAL	S 0,995/ELYC.EVAL	ELYC
Temperature **(1)**	Cel	/ELYC.T	S 35/ELYC.T	ELYC
Solvent		/ELYC.SOL	S NITROMETHANE/ELYC.SOL	ELYC
Remark		/ELYC.REM	S CONDUCTIVITY/ELYC.REM	ELYC
Comment		/ELYC.COM	S ACETATE/ELYC.COM	ELYC
Cross-Section				
Comment **(2)**	-	/XS.COM	S ELEKTRONEN/XS.COM	XS
Description	-	/XS.KW	S COLLISION CROSS-SECTION/XS.KW	XS

(1) Numeric search field that may be searched using numeric operators or ranges.
(2) Input partly in German.

Physical and Mechanical Properties

Search Field Name	Default Units	Fields Searched	Search Examples	Display Codes
Compressibility				
Comment **(1)**	-	/CMP.COM	S LIQUID/CMP.COM	CMP
Description	-	/CMP.KW	S ADIABATIC COMPRESSIBILITY/ CMP.KW	CMP
Density of the Liquid (2)	g*cm**3	/DEN	S 1/DEN	DEN
Comment **(1)**	-	/DEN.COM	S ALCOHOL/DEN.COM	DEN
Measurement Temperature **(2)**	Cel	/DEN.T	S 20/DEN.T	DEN
Reference Temperature **(2)**	Cel	/DEN.RT	S 10/DEN.RT	DEN
Mechanical Property				
Comment **(1)**	-	/MEC.COM	S HANDBOOK/MEC.COM	MEC
Description	-	/MEC.KW	S VISCOSITY/MEC.KW	MEC
Acoustic Property				
Comment **(1)**	-	/SOUND.COM	S METHYL/SOUND.COM	SOUND
Description	-	/SOUND.KW	S VELOCITY OF SOUND/SOUND.KW	SOUND
Surface Tension (2)	g/s**2	/ST	S 1.9-2/ST	ST
Comment **(1)**	-	/ST.COM	HEXENE/ST.COM	ST
Temperature **(2)**	Cel	/ST.T	S 20-22/ST.T	ST
Thermal Expansion		/TEC		TEC
Temperature (2)	Cel	/TEC.T	S –233/TEC.T	TEC
Coefficient (2)	-	/TEC.VAL	S 0.99/TEC.VAL	TEC
Keyword	-	/TEC.KW	S CUBIC EXPANSION/TEC.KW	TEC
Further Information (Physical and Chemical Properties) **(3)**	**-**	-	S FINFO/FA	FINFO

(1) Input partly in German.
(2) Numeric search field that may be searched using numeric operators or ranges.
(3) Field contains citations concerning further physical and chemical properties not covered in detail in ReaxsyFile. Only available via Field Availability (/FA).

Multi-Component Systems (MCS)

Search Field Name	Default Units	Fields Searched	Search Examples	Display Codes
Adsorption (MCS)				
Comment **(1)**	-	/ADSM.COM	S ISOMERS/ADSM.COM	ADSM
Description	-	/ADSM.KW	S ENTHALPY OF ADSORPTION/ADSM.KW	ADSM
Partner **(1)**	-	/ADSM.PA	S TRITON X-100/ADSM.PA	ADSM
Partner AN **(2)**	none	/ADSM.PAAN	S 2822009/ADSM.PAAN	ADSM
Pressure **(2)**	Torr	/ADSM.P	S 0.5-20/ADSM.P	ADSM
Solvent	-	/ADSM.SOL	S H2SO4/ADSM.SOL	ADSM
Temperature **(2)**	Cel	/ADSM.T	S 100/ADSM.T	ADSM
Association (MCS)	-			ASSM
Comment **(1)**	-	/ASSM.COM	S ACIDIC/ASSM.COM	ASSM
Description	-	/ASSM.KW	S ASSOCIATION WITH COMPOUND/ ASSM.KW	ASSM
Partner **(1)**	-	/ASSM.PA	S IMIDAZOLE/ASSM.PA	ASSM
Partner AN **(1)**	none	/ASSM.PAAN	S 54438/ASSM.PAAN	ASSM
Pressure **(2)**	Torr	/ASSM.P	S 0.5-1.5/ASSM.P	ASSM
Solvent	-	/ASSM.SOL	S CDCL3/ASSM.SOL	ASSM
Temperature **(2)**	Cel	/ASSM.T	S ASSM.T>100	ASSM
Azeotrope (MCS)				
Azeotrope Partner **(1)**	-	/AZE.PA	S DODECANE/AZE.PA	AZE
Azeotropes AN **(2)**	none	/AZE.PAAN	S 1697175/AZE.PAAN	AZE
Comment **(1)**	-	/AZE.COM	S NEGATIVE/AZE.COM	AZE
Concentrations	-	/AZE.C	S 71/AZE.C	AZE
Pressure **(2)**	Torr	/AZE.P	S 199.8/AZE.P	AZE
Temperature **(2)**	Cel	/AZE.T	S 20-25/AZE.T	

Multi-Component Systems (MCS) (cont'd)

Search Field Name	Default Units	Fields Searched	Search Examples	Display Codes
Boundary Surface Phenomena				
Comment **(1)**	-	/BSPM.COM	S HEXAN/BSPM.COM	BSPM
Description	-	/BSPM.KW	S SURFACE TENSION/BSPM.KW	BSPM
Partner **(1)**	-	/BSPM.PA	S METHANOL/BSPM.PA	BSPM
Partner AN **(2)**	none	/BSPM.PAAN	S 1098229/BSPM.PAAN	BSPM
Pressure **(2)**	Torr	/BSPM.P	S 0-750060/BSPM.P	BSPM
Solvent	-	/BSPM.SOL	S H2O/BSPM.SOL	BSPM
Temperature **(2)**	Cel	/BSPM.T	S 100/BSPM.T	BSPM
Complex Phase Equilibria				
Comment **(1)**	-	/CPEM.COM	S DEPENDENCE/CPEM.COM	CPEM
Description	-	/CPEM.KW	S PHASE EQUILIBRIUM/CPEM.KW	CPEM
Partner **(1)**	-	/CPEM.PA	S (XYLENE AND WATER)/CPEM.PA	CPEM
Partner AN **(2)**	none	/CPEM.PAAN	S 1421310/CPEM.PAAN	CPEM
Pressure **(2)**	Torr	/CPEM.P	S 30000-40000/CPEM.P	CPEM
Solvent	-	/CPEM.SOL	S H2O/CPEM.SOL	CPEM
Temperature **(2)**	Cel	/CPEM.T	S 20/CPEM.T	CPEM
Critical Micelle Concentration (MCS) (2)	g/L	/CMC	S 0.025/CMC	CMC
Comment **(1)**	-	/CMC.COM	S MICELLE/CMC.COM	CMC
Solvent	-	/CMC.SOL	S H2O/CMC.SOL	CMC
Temperature **(2)**	Cel	/CMC.T	S 0.025/CMC AND 40/CMC.T	CMC
Electrical Data				
Comment **(1)**	-	/EDM.COM	S CONCENTRATION/EDM.COM	EDM
Description	-	/EDM.KW	S DIELECTRIC CONSTANT/EDM.KW	EDM
Partner **(1)**	-	/EDM.PA	S TETRATRIACONTANOL/EDM.PA	EDM
Partner AN **(2)**	none	/EDM.PAAN	S 1798829/EDM.PAAN	EDM
Temperature **(2)**	Cel	/EDM.T	S 20-30/EDM.T	EDM
Energy Data (MCS)				
Comment **(1)**	-	/ENEM.COM	S CYCLOHEXANON/ENEM.COM	ENEM
Description	-	/ENEM.KW	S ENTHALPY OF SOLUTION/ENEM.KW	ENEM
Partner **(1)**	-	/ENEM.PA	S 1,3-BUTANEDIOL/ENEM.PA	ENEM
Partner AN **(2)**	-	/ENEM.PAAN	S 969148/ENEM.PAAN	ENEM
Pressure **(2)**	Torr	/ENEM.P	S 2-20/ENEM.P	ENEM
Solvent	-	/ENEM.SOL	S TOLUENE/ENEM.SOL	ENEM
Temperature **(2)**	Cel	/ENEM.T	S 25-30/ENEM.T	ENEM
Henry Constant (MCS) (2)	PA*M**3 /mOL	/HNC	S 20-30/HNC	HNC
Comment **(1)**	-	/HNC.COM	S CONSTANT/HNC.COM	HNC
Log Henry Constant **(2)**	-	/HNC.LOG	S -5.72/HNC.LOG	HNC
Solvent	-	/HNC.SOL	S H2O/HNC.SOL	HNC
Temperature **(2)**	Cel	/HNC.T	S 25/HNC.T	HNC
Liquid/Liquid System				
Comment **(1)**	-	/LLSM.COM	S HEPTAN/LLSM.COM	LLSM
Description	-	/LLSM.KW	S LIQUID/LIQUID PHASE DIAGRAM/LLSM.KW	LLSM
Partner **(1)**	-	/LLSM.PA	S TETRACHLOROMETHANE/LLSM.PA	LLSM
Partner AN	-	/LLSM.PAAN	S 1098295/LLSM.PAAN	LLSM
Pressure **(2)**	Torr	/LLSM.P	S 0-10000/LLSM.P	LLSM
Solvent	-	/LLSM.SOL	S DIMETHYLSULFOXIDE/LLSM.SOL	LLSM
Temperature **(2)**	Cel	/LLSM.T	S 5-10/LLSM.T	LLSM
Liquid/Solid System				
Comment **(1)**	-	/LSSM.COM	S HOMOLOGE/LSSM.COM	LSSM
Description	-	/LSSM.KW	S PHASE TRANSITION TEMPERATURE?/LSSM.KW	LSSM

Multi-Component Systems (MCS) (cont'd)

Search Field Name	Default Units	Fields Searched	Search Examples	Display Codes
Partner **(1)**	-	/LSSM.PA	S STRYCHNIDIN-10-ONE/LSSM.PA	LSSM
Pressure **(2)**	Torr	/LSSM.P	S 0-20000/LSSM.P	LSSM
Partner AN **(2)**	-	/LSSM.PAAN	S 52979/LSSM.PAAN	LSSM
Partner AN **(2)**	-	/LVSM.PAAN	S 506007/LVSM.PAAN	LVSM
Pressure **(2)**	Torr	/LVSM.P	S 19000-90000/LVSM.P	LVSM
Solvent		/LVSM.SOL	S PROPAN-1-OL/LVSM.SOL	LVSM
Temperature **(2)**		/LVSM.T	S 120/LVSM.T	LVSM
Mechanical & Physical Property (MCS)				
Comment **(1)**	-	/MECM.COM	S DIAGRAM/MECM.COM	MECM
Description	-	/MECM.KW	S ISOTHERMAL COMPRESS?/MECM.KW	MECM
Partner **(1)**	-	/MECM.PA	S OCTANE-2-OL/MECM.PA	MECM
Partner AN **(2)**	-	/MECM.PAAN	S 1697461/MECM.PAAN	MECM
Pressure **(2)**	Torr	/MECM.P	S 1-10/MECM.P	MECM
Solvent	-	/MECM.SOL	S HCL/MECM.SOL	MECM
Temperature	Cel	/MECM.T	S 25-65/MECM.T	MECM
Optical Data (MCS)				
Comment		/ODM.COM	S STUDY/ODM.COM	ODM
Description	-	/ODM.KW	S KERR CONSTANT/ODM.KW	ODM
Partner **(1)**	-	/ODM.PA	S PHENOL/ODM.PA	ODM
Partner AN **(2)**	-	/ODM.PAAN	S 969616/ODM.PAAN	ODM
Partition Constant (Octan-1-o1/Water) (2)	-	/POW	S 1.5-2/POW	POW
Comment		/POW.COM	S BUFFER/POW.COM	POW
log POW **(2)**	-	/POW.LOG	S -0.9- -0.7/POW.LOG	POW
Temperature **(2)**	Cel	/POW.T	S 20/POW.T	POW
Solubility (MCS)	g/L	/SLB	S 0.001/SLB	SLB
Comment **(1)**	-	/SLB.COM	S PH/SLB.COM	SLB
Ratio of Solvents	-	/SLB.RAT	S (6 (P) 1)/SLB.RAT	SLB
Saturation	-	/SLB.SAT	S IN PURE SOLVENT/SLB.SAT	SLB
Solvent	-	/SLB.SOL	S DIETHYL ETHER/SLB.SOL	SLB
Temperature **(2)**	Cel	/SLB.T	S 10/SLB.T	SLB
Solubility Product (MCS) (2)	-	/SLBP	S SLBP<0.00002	SLBP
Comment **(1)**	-	/SLBP.COM	S NACL04/SLBP.COM	SLBP
Ratio of Solvents	-	/SLBP.RAT	S (30 (P) PERCENT)/SLBP.RAT	SLBP
Solvent	-	/SLBP.SOL	S H2O/SLBP.SOL	SLBP
Temperature **(2)**	Cel	/SLBP.T	S 25/SLBP.T	SLBP
Solution Behaviour (MCS)				
Comment **(1)**	-	/SOLM.COM	S PRESSURE/SOLM.COM	SOLM
Description	-	/SOLM.KW	S MISCIBILITY/SOLM.KW	SOLM
Partner **(1)**		/SOLM.PA	S XYLITOL/SOLM.PA	SOLM
Partner AN **(2)**		/SOLM.PAAN	S 2049713/SOLM.PAAN	SOLM
Pressure	Torr	/SOLM.P	S 780-850/SOLM.P	SOLM
Solvent		/SOLM.SOL	S TETRAHYDROFURAN/SOLM.SOL	SOLM
Temperature **(2)**		/SOLM.T	S 20/SOLM.T	SOLM
Transport Phenomena (MCS)				
Comment **(1)**	-	/TRAM.COM	S HELIUM/TRAM.COM	TRAM
Description		/TRAM.KW	S DYNAMIC VISCOSITY/TRAM.KW	TRAM
Partner **(1)**	-	/TRAM.PA	S ETHANOL/TRAM.PA	TRAM
Partner AN **(2)**	-	/TRAM.PAAN	S 1718733/TRAM.PAAN	TRAM
Pressure **(2)**	Torr	/TRAM.P	S 0-800000/TRAM.P	TRAM
Solvent	-	/TRAM.SOL	S PYRIDINE/TRAM.SOL	TRAM
Temperature **(2)**	Cel	/TRAM.T	S 9.9/TRAM.T	TRAM

(1) Input partly in German.
(2) Numeric search field that may be searched using numeric operators or ranges.

Optical Properties

Search Field Name	Default Units	Fields Searched	Search Examples	Display Codes
Circular Dichroism				
Comment **(1)**	-	/CDIC.COM	S IPROH/CDIC.COM	CDIC
Solvent	-	/CDIC.SOL	S CHCL3/CDIC.SOL	CDIC
Mutarotation (2)	deg	/MUT	S 10-20/MUT	MUT
Comment **(1)**	-	/MUT.COM	S BETA/MUT.COM	MUT
Concentration	-	/MUT.C	S 0.7 G/100ML/MUT.C	MUT
Length of Path **(2)**	cm	/MUT.LEN	S MUT.LEN>10	MUT
Solvent	-	/MUT.SOL	S H2O/MUT.SOL	MUT
Temperature **(2)**	Cel	/MUT.T	S 21/MUT.T	MUT
Time	-	/MUT.TIM	S 300MUT.TIM	MUT
Type	-	/MUT.TYP	S M/MUT.TYP	MUT
Wavelength **(2)**		/MUT.W	S 589/MUT.W	MUT
Optics				
Comment **(1)**	-	/OPT.COM	S ACETON/OPT.COM	OPT
Description	-	/OPT.KW	S LINEAR DICHROISM/OPT.KW	OPT
Optical Rotatory Dispersion				
Comment **(1)**	-	/ORD.COM	S CYCLOHEXANOL/ORD.COM	ORD
Solvent	-	/ORD.SOL	S ETHANOL/ORD.SOL	ORD
Optical Rotatory Power (2)	deg	/ORP	S 39.65-40/ORP	ORP
Comment **(1)**	-	/ORP.COM	S ACETAMIDE/ORP.COM	ORP
Concentration	-	/ORP.C	S 1 MOL/L/ORP.C	ORP
Length of Path **(2)**	cm	/ORP.LEN	S 10/ORP.LEN	ORP
Solvent	-	/ORP.SOL	S BENZENE/ORP.SOL	ORP
Temperature **(2)**	Cel	/ORP.T	S 20/ORP.T	ORP
Type	-	/ORP.TYP	S ALPHA/ORP.TYP	ORP
Wavelength **(2)**	nm	/ORP.W	S 578/ORP.W	ORP
Refractive Index (2)	-	/RI	S 1.00056/RI	RI
Comment **(1)**	-	/RI.COM	S BENTYL/RI.COM	RI
Temperature **(2)**	Cel	/RI.T	S 0/RI.T	RI
Wavelength **(2)**	nm	/RI.W	S 586/RI.W	RI

(1) Input partly in German.
(2) Numeric search field that may be searched using numeric operators or ranges

Patent Specific Data

Search Field Name	Fields Searched	Search Examples	Display Codes
Patent Specific Data			PSD
Location in Patent	/PSD.LCN	S CLAIM/PSD.LCN	PSD
Prophetic Substance	/PSD.PRC	S CATALYST/PSD.PRC	PSD
Related Markush Structure	/AN	S 11337539/AN	IDE

Pharmacological and Ecological Data

Search Field Name	Default Units	Fields Searched	Search Examples	Display Codes
ECOLOGICAL DATA				
Abiotic Degradation, Hydrolysis				
Degradation Product AN **(1)**	-	/ECDH.AN	S 647116/ECDH.AN	ECDH
Concentration	-	/ECDH.C	S 0.21 PPM/ECDH.C	ECDH
Comment **(2)**	-	/ECDH.COM	S (FURTHER (W) DEGRADATION (W) PRODUCT?)/ECDH.COM	ECDH
Degradation Rate	-	/ECDH.D	S 100/ECDH.D	ECDH
Degradation Product **(2)**	-	/ECDH.DP	S OCTACHLORODIBENZOBENZOFURAN/ECDH.DP	ECDH
Exposure Period	-	/ECDH.EX	S HECDH.EX	ECDH
Half-life Time	-	/ECDH.H	S 0.5/ECDH.H	ECDH
Method, Remarks	-	/ECDH.MR	S GC/ECDH.MR	ECDH
pH-Value	-	/ECDH.PH	S 1.01/ECDH.PH	ECDH
Rate Constant	-	/ECDH.RC	S 1.15 PER HOUR/ECDH.RC	ECDH
Temperature	-	/ECDH.T	S 10/ECDH.T	ECDH
Type	-	/ECDH.TYP	S OXIDATION/ECDH.TYP	ECDH
Abiotic Degradation, Photolysis				
Degradation Product AN **(1)**	-	/ECDP.AN	S 1446588/ECDP.AN	ECDP
Concentration	-	/ECDP.C	S 5.9 PPM/ECDP.C	ECDP
Comment **(2)**	-	/ECDP.COM	S (DEGRADATION (W) PRODUCT?) /ECDP.COM	ECDP
Degradation Rate	-	/ECDP.D	S 80/ECDP.D	ECDP
Degradation Product **(2)**		/ECDP.DP	S HEXACHLORO/ECDP.DP	ECDP
Exposure Period	-	/ECDP.EX	S 3 H?/ECDP.EX	ECDP
Half-life Time	-	/ECDP.H	S 1/ECDP.H	ECDP
Method, Remarks	-	/ECDP.MR	S H2O2/ECDP.MR	ECDP
pH-Value	-	/ECDP.PH	S PHOTOOXIDATION/ECDP.TYP (P) 2.8/ECDP.PH	ECDP
Rate Constant	-	/ECDP.RC	S 0.090 – 0.245 MIN-1/ECDP.RC	ECDP
Temperature	-	/ECDP.T	S 600/ECDP.T	ECDP
Type	-	/ECDP.TYP	S PHOTOLYSIS/ECDP.TYP	ECDP
Biodegradation				
Comment **(2)**	-	/BIOD.COM	S (FURTHER (W) DEGRADATION (W) PRODUCT)/BIOD.COM	BIOD
Concentration	-	/BIOD.C	S 1 G/L/BIOD.C	BIOD
Degradation Product **(2)**	-	/BIOD.DP	S (CARBOXYLATED (W) ALIPHATIC (W) ALCOHOL)/BIOD.DP	BIOD
Degradation Product AN	-	/BIOD.AN	S 8697186/BIOD.AN	BIOD
Degradation Rate	-	/BIOD.D	S 28 - 36/BIOD.D	BIOD
Exposure Period	-	/BIOD.EX	S 8 W?/BIOD.EX	BIOD
Half-life Time	-	/BIOD.H	S 40?/BIOD.H	BIOD
Inoculum	-	/BIOD.IN	S (ACTIVATED (W) SLUDGE)/BIOD.IN	BIOD
Method, Remarks	-	/BIOD.MR	S (SEWAGE (W) TREATMENT)/BIOD.MR	BIOD
Temperature	-	/BIOD.T	S 20/BIOD.T	BIOD
Type	-	/BIOD.TYP	S AEROBIC/BIOD.TYP	BIOD
Biological Behaviour				
Accumulation Half-Life Time	-	/BIO.A	S 5 D?/BIO.A	BIO
Accumulation Rate Constant	-	/BIO.AR	S 0.882 PER HOUR/BIO.AR	BIO
Bioconcentration Factor (F)	-	/BIO.BC	S 0.03/BIO.BC	BIO
Biomagnification	-	/BIO.MAG	S 20/BIO.MAG	BIO
Biomonitoring	-	/BIO.MON	S LEUKOCYTES/BIO.MON	BIO
Concentration	-	/BIO.C	S 0.03 - 58 .MY.G/L/BIO.C	BIO
Elimination Half-Life Time	-	/BIO.H	S 28 D?/BIO.H	BIO

Pharmacological and Ecological Data (cont'd)

Search Field Name	Default Units	Fields Searched	Search Examples	Display Codes
Elimination Rate Constant	-	/BIO.ER	S 1.1 PER DAY/BIO.ER	BIO
Exposure Period	-	/BIO.EX	S 5 D?/BIO.EX	BIO
Log BCF	-	/BIO.LOG	S 8.2/BIO.LOG	BIO
Media	-	/BIO.ME	S FOOD/BIO.ME	BIO
Method, Remarks	-	/BIO.MR	S (FISH (W) BRAIN (W) ACETYLCHOLINESTERASE)/BIO.MR	BIO
Species	-	/BIO.SP	S (SALMO (W) SOLAR)/BIO.SP	BIO
Temperature **(1)**	C	/BIO.T	S 10-15/BIO.T	BIO
Concentration in Environment				
Background Concentration	-	/COEV.BC	S (FAT (W) BASIS)/COEV.BC	COEV
Contamination Concentration	-	/COEV.CC	S 0 - 20.420 MG/KG DRY WT/COEV.CC	COEV
Location	-	/COEV.LO	S LAKE MICHIGAN/COEV.LO	COEV
Media	-	/COEV.ME	S TOLUENE/CN AND SOIL/COEV.ME	COEV
Method, Remarks	-	/COEV.MR	S (FISH? (S) CAPTURE? (S) APRIL (S)1996)/COEV.MR	COEV
Species	-	/COEV.SP	S FISH/COEV.SP	COEV
Ecological Mobility: Transport and Distribution				
Media	-	/ECTD.ME	S WATER - AIR/ECTD.ME	ECTD
Method, Remarks	-	/ECTD.MR	S (SOLID (W) PHASE)/ECTD.MR	ECTD
Results	-	/ECTD.RE	S (SORPTION (W) ISOTHERM)/ECTD.RE	ECTD
Type	-	/ECTD.TYP	S ADSORPTION/ECTD.TYP	ECTD
Ecotoxicology				
Comment **(2)**	-	/ECTOX.COM	S (FURTHER(W)METABOL?)/ECTOX.COM	ECTOX
Concentration	-	/ECTOX.C	S 3 - 10 .MY.G/L/ECTOX.C	ECTOX
Effect	-	/ECTOX.E	S ABSORPTION/ECTOX.E	ECTOX
Endpoint of Effect	-	/ECTOX.EP	S (GROWTH(W)INHIBITION)/ECTOX.EP	ECTOX
Exposure Period	-	/ECTOX.EX	S 10 D?/ECTOX.EX	ECTOX
Further Details	-	/ECTOX.FD	S TEQ/ECTOX.FD	ECTOX
Kind of Dosing	-	/ECTOX.KD	S SOIL/ECTOX.KD	ECTOX
Metabolite **(2)**	-	/ECTOX.META	S METHYL BUTYLHEXANOL/ECTOX.META	ECTOX
Metabolite AN **(1)**	-	/ECTOX.AN	S 2242347/ECTOX.AN	ECTOX
Method	-	/ECTOX.MR	S (CHOICE (W) BIOASSAY)/ECTOX.MR	ECTOX
Results	-	/ECTOX.RE	S (EFFECTS (2W) OVARIES)/ECTOX.RE	ECTOX
Route of Application	-	/ECTOX.RA	S PERORAL/ECTOX.RA	ECTOX
Sex	-	/ECTOX.S	S FEMALE/ECTOX.S	ECTOX
Species or Test-System	-	/ECTOX.SP	S (EISENIA (W) FOETIDA)/ECTOX.SP	
Type	-	/ECTOX.TYP	S LC50/ECTOX.TYP	ECTOX
Value of Type	-	/ECTOX.V	S CA. 0.2 NKAT/MG PROTEIN/ECTOX.V	ECTOX
Exposure Assessment				
Exposure	-	/EXCA.HE	S (DISTRIBUTION(S)WATER)/EXCA.HE	EXCA
Sources	-	/EXCA.SO	S OIL/EXCA.SO	EXCA
Oxygen Demand				
Concentration	-	/EOD.C	S 1.5 G/EOD.C	EOD
Method, Remarks	-	/EOD.MR	S (STANDARD (2W) METHOD?)/EOD.MR	EOD
Oxygen Demand	-	/EOD.D	S 290.7/EOD.D	EOD
Ratio BOD5/COD	-	/EOD.RAT	S 0.98/EOD.RAT	EOD
Related to	-	/EOD.RE	S DOC/EOD.RE	EOD
Type	-	/EOD.TYP	S BOD10/EOD.TYP	EOD

Pharmacological and Ecological Data (cont'd)

Search Field Name	Default Units	Fields Searched	Search Examples	Display Codes
Stability in Soil				
Caution Exchange Rate	-	/ECS.CE	S "11.45 C MOL (P + T) KG-1"/ECS.CE	ECS
Concentration	-	/ECS.C	S 50 MG/KG/ECS.C	ECS
Dissipation	-	/ECS.D	S 33/ECS.D	ECS
Dissipation Time 50	-	/ECS.5	S 1332/ECS.5	ECS
Dissipation Time 90	-	/ECS.9	S 25 D/ECS.9	ECS
Exposure Period	-	/ECS.EX	S (64(W)D?)/ECS.EX	ECS
Humidity	-	/ECS.HU	S 0.3 - 2.7 PERCENT/ECS.HU	ECS
Method, Remarks		/ECS.MR	S (SOIL (2W) HOLIDAY(W)BEACH/ECS.MR	ECS
Microbial Biomass	-	/ECS.MB	S 9.8E7 CFU/G/ECS.MB	ECS
Organic Carbon	-	/ECS.OC	S (50 (W) PERCENT)/ECS.OC	ECS
pH-Value **(1)**	-	/ECS.PH	S 2-5/ECS.PH	ECS
Temperature **(1)**	C	/ECS.T	S 20>ECS.T	ECS
Type		/ECS.TYP	S (SANDY (W) LOAM)/ECS.TYP	ECS
PHARMACOLOGICAL DATA				
Concentration	-	/PHARM.C	S 10 MG/KG/PHARM.C	PHARM
Comment **(2)**	-	/PHARM.COM	S ANTIFUNGAL/PHARM.COM	PHARM
Effect	-	/PHARM.E	S ACUTE TOXICITY ORAL/PHARM.E	PHARM
Endpoint of Effect	-	/PHARM.EP	S (CELL (W) DEATH)/PHARM.EP	PHARM
Exposure Period	-	/PHARM.EX	S Y/PHARM.EX	PHARM
Further Details	-	/PHARM.FD	S ELECTROPHYSIOLOGICAL/PHARM.FD	PHARM
Half-life Time	-	/PHARM.H	S "2"/PHARM.H	PHARM
Kind of Dosing	-	/PHARM.KD	S DAILY/PHARM.KD	PHARM
Metabolite **(2)**	-	/PHARM.META	S PYREN/PHARM.META	PHARM
Metabolite AN **(1)**	-	/PHARM.AN	S 8407954/PHARM.AN	PHARM
Method	-	/PHARM.MR	S (IN (W) VITRO)/PHARM.MR	PHARM
Results	-	/PHARM.RE	S DOSE10/PHARM.RE	PHARM
Route of Application	-	/PHARM.RA	S EPICUTANEOUS/PHARM.RA	PHARM
Sex	-	/PHARM.S	S FEMALE/PHARM.S	PHARM
Species or Test-System	-	/PHARM.SP	S BACTERIA/PHARM.SP	PHARM
Type	-	/PHARM.TYP	S BENZENE/CN AND LD50/PHARM.TYP	PHARM
Value of Type	-	/PHARM.V	S EC50/PHARM.TYP (P) 0.1 MG/L/PHARM.V	PHARM
LABORATORY USE AND HANDLING				
Use of Compound				
Comment **(2)**	-	/USC.COM	S LIGHT/USC.COM	USC
Laboratory Use and Handling **(2)**	-	/USC.LH	S (POLYMERIC(2W)SURFACTANT)/USC.LH	USC
Use Pattern	-	/USC.PT	S (DETECTION (2W) PENICILLIN (2W) MILK)/USC.PT	USC

(1) Numeric search field that may be searched using numeric operators or ranges.
(2) Input partly in German.

Safety Data

Search Field Name	Default Units	Fields Searched	Search Examples	Display Codes
Flash Point	CEL	/FP.T	S 105/FP.T	FP
Type of Test **(1)**	-	/FP.TYP	S DIN/FP.TYP	FP
Explosion Limits	Vol%	/EL.LV	S 1.8/EL.LV	EL

(1) Numeric search field that may be searched using numeric operators or ranges.

Spectroscopic Data

Search Field Name	Default Units	Fields Searched	Search Examples	Display Codes
ESR Data				
Comment **(1)**	-	/ESR.COM	S (INORGANIC(P)COMPOUNDS)/ESR.COM	ESR
Coupling Nuclei	-	/ESR.NUI	S 2D/ESR.NUI	ESR
Description	-	/ESR.KW	S SPECTRUM/ESR.KW	ESR
Solvents	-	/ESR.SOL	S CH2CL2/ESR.SOL	ESR
Temperature **(2)**	Cel	/ESR.T	S 19-20/ESR.T	ESR
Fluorescence				
Comment **(1)**	-	/FLU.COM	S HELIUM/FLU.COM	FLU
Description	-	/FLU.KW	S MAXIMA/FLU.KW	FLU
Solvent	-	/FLU.SOL	S ACETONITRILE/FLU.SOL	FLU
Temperature **(2)**	Cel	/FLU.T	S 25/FLU.T	FLU
Infrared Spectrum				
Comment **(1)**	-	/IR.COM	S PH/IR.COM	IR
Description	-	/IR.KW	S FINE STRUCTURE OF IR BANDS/IR.KW	IR
Solvent	-	/IR.SOL	S CHCL 3/IR.SOL	IR
Temperature **(2)**	Cel	/IR.T	S IR.T>50	IR
Original Text		/IR.TXT	S MAXIMUM/IR.TXT	IR
Luminescence				
Comment **(1)**	-	/LUM.COM	S (TEMPERATURE(P)DEPENDE?)/LUM.COM	LUM
Description	-	/LUM.KW	S LUMINESCENCE QUENCHING/LUM.KW	LUM
Mass Spectrum				
Comment **(1)**	-	/MS.COM	S METASTABLE/MS.COM	MS
Description	-	/MS.KW	S FRAGMENTATION PATTERN/MS.KW	MS
Nuclear Magnetic Resonance				
Comment **(1)**	-	/NMR.COM	S (AMBIENT (P) TEMPERATURE)/NMR.COM	NMR
Coupling Nuclei	-	/NMR.NUI	S (1H and 13C)/NMR.NUI	NMR
Description	-	/NMR.KW	S 2D-NMR/NMR.KW	NMR
Frequency **(2)**	-	/NMR.F	S 50/NMR.F	NMR
Nucleus	-	/NMR.NUC	S 31P/NMR.NUC	NMR
Solvents	-	/NMR.SOL	S CDCL3/NMR.SOL	NMR
Temperature **(2)**	Cel	/NMR.T	S 20-22/NMR.T	NMR
Original Text		/NMR.TXT	S SHIFTS/NMR.TXT	NMR
Nuclear Quadrupole Resonance				
Comment **(1)**	-	/NQR.COM	S (NQR (P) ABSORPTION)/NQR.COM	NQR
Description	-	/NQR.KW	S NUCLEAR QUADRUPOLE RESONANCE/NQR.KW	NQR
Nucleus	-	/NQR.NUC	S 35CL/NQR.NUC	NQR
Other Spectroscopic Methods				
Comment **(1)**	-	/OSM.COM	S SHIFTS/OSM.COM	OSM
Description	-	/OSM.KW	S PHOTOELECTRON SPECTRUM/OSM.KW	OSM
Nucleus		/OSM.NUC	S FE/OSM.NUC	OSM
Phosphorescence				
Comment **(1)**	-	/PHO.COM	S ISOPENTAN/PHO.COM	PHO
Description	-	/PHO.KW	S TRIPLET STATE LIFETIME/PHO.KW	PHO
Solvent	-	/PHO.SOL	S ETHANOL/PHO.SOL	PHO
Temperature **(2)**	Cel	/PHO.T	S 25/PHO.T	PHO
Raman Spectrum				
Comment **(1)**	-	/RAS.COM	S (GASEOUS (P) MATRIX)/RAS.COM	RAS
Description	-	/RAS.KW	S RAMAN INTENSITIES/RAS.KW	RAS
Solvent	-	/RAS.SOL	S KBR/RAS.SOL	RAS

Spectroscopic Data (cont'd)

Search Field Name	Default Units	Fields Searched	Search Examples	Display Codes
Rotational Spectrum				
Comment **(1)**	-	/ROT.COM	S ROTATIONSDISPERSION/ROT.COM	ROT
Description	-	/ROT.KW	S ROTATIONAL SPECTRUM/ROT.KW	ROT
UV and Visible Spectrum				
Absorption Maxima **(2)**	nm	/UVS.AM	S 139-139.1/UVS.AM	UVS
Comment **(1)**	-	/UVS.COM	S (ACIDIC (P) SOLUTION)/UVS.COM	UVS
Description		/UVS.KW	S ABSORPTION MAXIMA/UVS.KW	UVS
Ext./Abs. Coef. **(2)**	1/mol* cm	/UVS.EAC	S 4.4/UVS.EAC	UVS
Solvent		/UVS.SOL	S CYCLOHEXANE/UVS.SOL	UVS

(1) Input partly in German.
(2) Numeric search field that may be searched using numeric operators or ranges.

Structure and Energy Parameters

Search Field Name	Default Units	Fields Searched	Search Examples	Display Codes
Conformation				
Object of Investigation	-	/CNF.OBJ	S CONFORMER EQUILIBRIUM/CNF.OBJ	CNF
Dipole Moment				
Comment **(1)**	-	/DM.COM	S CONCENTRATION/DM.COM	DM
Description	-	/DM.KW	S QUADRUPOLE MOMENT/DM.KW	DM
Moment **(2)**	D	/DM	S 1-1.22/DM	DM
Method	-	/DM.MET	S DIELECTRIC/DM.MET	DM
Solvent	-	/DM.SOL	S CCL4/DM.SOL	DM
Temperature **(1)**	Cel	/DM.T	S 20>DM.T	DM
Electrical Polarizability				
Comment **(1)**	-	/POL.COM	S (TIME (P) DEPENDENCE)/POL.COM	POL
Description	-	/POL.KW	S ELECTRON POLARIZATION/POL.KW	POL
Electron Binding				
Comment **(1)**	-	/CIP.COM	S (EXCITED (P) STATE)/CIP.COM	CIP
Description	-	/CIP.KW	S ELECTRON AFFINITY/CIP.KW	CIP
Energy Barrier of Conformation (2)				
Barrier Type	-	/EBC.TYP	S CF3/EBC.TYP	EBC
Comment **(1)**	-	/EBC.COM	S ROTATION/EBC.COM	EBC
Solvent	-	/EBC.SOL	S TOLUENE/EBC.SOL	EBC
Energy of Dissociation (2)	J/mol	/EDIS	S 12000-14000/EDIS	EDIS
Bond Type	-	/EDIS.TYP	S (P (P) H)/EDIS.TYP	EDIS
Comment **(1)**	-	/EDIS.COM	S DISSOZIATIONSENERGIE/EDIS.COM	EDIS
Ionization Potential (2)	eV	/IP	S 7-8/IP	IP
Comment **(1)**		/IP.COM	S VERTICAL/IP.COM	IP
Method		/IP.MET	S PHOTOIONIZATION/IP.MET	IP

Structure and Energy Parameters (cont'd)

Search Field Name	Default Units	Fields Searched	Search Examples	Display Codes
Interatomic Distance and Angle				
Comment **(1)**	-	/GEO.COM	S METHOD/GEO.COM	GEO
Description	-	/GEO.KW	S "INTERATOMIC DISTANCES AND ANGLES"/GEO.KW	GEO
Molecular Deformation				
Comment **(1)**	-	/DFM.COM	S ACETONITRIL?/DFM.COM	DFM
Description	-	/DFM.KW	S FREQUENZ/DFM.KW	DFM

(1) Numeric search field that may be searched using numeric operators or ranges.
(2) Input partly in German.

State of Aggregation

Search Field Name	Default Units	Fields Searched	Search Examples	Display Codes
CRYSTALS				
Crystal Phase				
Comment **(2)**	-	/CRYPH.COM	S ANISOTROPIC/CRYPH.COM	CRYPH
Description	-	/CRYPH.KW	S CRYSTAL STRUCTURE?/CRYPH.KW	CRYPH
Temperature **(1)**	Cel	/CRYPH.T	S 14.85/CRYPH.T	CRYPH
Crystal Phase Transition Point (1)				
Change of Modification	-	/CTP.CM	S GLASS/CTP.CM	CTP
Comment **(2)**	-	/CTP.COM	S TRANSITION/CTP.COM	CTP
Crystal Property Description				
Colour & Other Properties	-	/CPD	S GLAS?/CPD	CDP
Comment	-	/CPD.COM	S HCL/CPD.COM	CPD
Point Group		/CPD.PGROUP	S C2/CPD.PGROUP	CPD
Crystal Space Group		/CSG	S 212/CSG	CSG
Comment **(2)**	-	/CSG.COM	S GROUP/CSG.COM	CSG
Crystal System		/CSYS	S MONOCLINIC/CSYS	CSYS
Comment **(2)**	-	/CSYS.COM	S (LABILE (P) FORM)/CSYS.COM	CSYS
Decomposition Point	Cel	/DP	S 0-10/DP	DP
Comment **(2)**	-	/DP.COM	S CRYSTALLIZATION/DP.COM	DP
Solvent for Crystallisation		/DP.CRSOL	S HEXANE/DP.CRSOL	DP
Solvent	-	/DP.SOL	S PROPAN-2-OL/DP.SOL	DP
Amount (1)		/DP.SOLM	S 13/DP.SOLM	DP
Density of the Crystal (1)	g/cm**3	/CDEN	S 5-5.1/CDEN	CDEN
Comment **(2)**	-	/CDEN.COM	S ORTHORHOMBISCH?/CDEN.COM	CDEN
Temperature **(1)**	Cel	/CDEN.T	S 293 K/CDEN.T	CDEN
Melting Point (1)	Cel	/MP	S 250-260/MP	MP
Comment **(2)**	-	/MP.COM	S DECOMPOSITION/MP.COM	MP
Solvent	-	/MP.SOL	S XYLENE/MP.SOL	MP
Sublimation Point (1)	Cel	/SP	S SP>=500	SP
Comment **(2)**	-	/SP.COM	S (MELTING (P) FORM)/SP.COM	SP
Pressure **(1)**	Torr	/SP.P	S 1/SP.P	SP
Triple Point (1)	Cel	/TP	S 20-21/TP	TP
Comment **(2)**	-	/TP.COM	S GASEOUS/TP.COM	TP

State of Aggregation (cont'd)

Search Field Name	Default Units	Fields Searched	Search Examples	Display Codes
GASES				
Critical Density (1)	g/cm**3	/CRD	S 0.2-0.2022/CRD	CRD
Critical Pressure (1)	Torr	/CRP	S CRP >760 MBAR	CRP
Comment **(2)**	-	/CRP.COM	S HANDBOOK/CRP.COM	CRP
Critical Temperature (1)	Cel	/CRT	S 500-600/CRT	CRT
Comment **(2)**	-	/CRT.COM	S NITRO/CRT.COM	CRT
Critical Volume (1)	cm**3/mol	/CRV	S 211/CRV	CRV
Comment **(2)**	-	/CRV.COM	S MOL/CRV.COM	CRV
Gas Phase				
Comment **(2)**	-	/GP.COM	S (SATURATED (P) LIQ?)/GP.COM	GP
Description	-	/GP.KW	S FUGACITY/GP.KW	GP
Vapour Pressure (1)	Torr	/VP	S 4-5/VP	VP
Comment **(2)**	-	/VP.COM	S EQUATION/VP.COM	VP
Temperature **(1)**	Cel	/VP.T	S VP>80 and VP.T<5	VP
LIQUIDS				
Boiling Point (1)	Cel	/BP	S BP> 200	BP
Comment **(2)**	-	/BP.COM	S BADTEMPERATUR/BP.COM	BP
Pressure **(1)**	Torr	/BP.P	S 1/BP.P	BP
Liquid Phase				
Comment **(2)**	-	/LIQPH.COM	S AETHANOL/LIQPH.COM	LIQPH
Description	-	/LIQPH.KW	S SELF-ASSOCIATION IN SOLUTION/LIQPH.KW	LIQPH
Transition Point of Liquid Modification (1)	Cel	/LPTP	S 20/LPTP	LPTP
Change of Modification	-	/LPTP.CM	S (NEMATIC(P)ISOTROPIC)/LPTP.CM	LPTP
Comment **(2)**	-	/LPTP.COM	S SOLID/LPTP.COM	LPTP

(1) Numeric search field that may be searched using numeric operators or ranges.
(2) Input partly in German.

Thermodynamic Properties

Search Field Name	Default Units	Fields Searched	Search Examples	Display Codes
Enthalpies of Other Transitions (1)	J/mol	/HPT	S 650-700/HPT	HPT
Comment **(2)**	-	/HPT.COM	S (HEXAGONAL (P) CUBIC)/HPT.COM	HPT
Enthalpy of Combustion (1)	J/mol	/HCOM	S HCOM>-100000	HCOM
Comment **(2)**	-	/HCOM.COM	S HEXAN/HCOM.COM	HCOM
Pressure **(1)**	Torr	/HCOM.P	S 1216/HCOM.P	HCOM
Temperature **(1)**	Cel	/HCOM.T	S 25/HCOM.T	HCOM
Enthalpy of Formation (1)	J/mol	/HFOR	S 808052/HFOR	HFOR
Comment **(2)**	-	/HFOR.COM	S KOBALT/HFOR.COM	HFOR
Pressure **(1)**	Torr	/HFOR.P	S 759-761/HFOR.P	HFOR
Temperature **(1)**	Cel	/HFOR.T	S HFOR.T<10	HFOR
Enthalpy of Fusion (1)	J/mol	/HFUS	S 1000-2000/HFUS	HFUS
Comment **(2)**	-	/HFUS.COM	S BETA/HFUS.COM	HFUS

Thermodynamic Properties (cont'd)

Search Field Name	Default Units	Fields Searched	Search Examples	Display Codes
Enthalpy of Hydrogenation (1)	J/mol	/HHDG	S 153362/HHDG	HHDG
Comment **(2)**	-	/HHDG.COM	S ENTHALPY/HHDG.COM	HHDG
Product AN	-	/HHDG.AN	S 2036502/HHDG.AN	HHDG
Product Name **(2)**	-	/HHDG.CN	S PHENYLCYCLOOCTANE/HHDG.CN	HHDG
Temperature	Cel	/HHDG.T	S 24.9/HHDG.T	HHDG
Enthalpy of Sublimation (1)	J/mol	/HSUB	S HSUB<40000	HSUB
Comment **(2)**	-	/HSUB.COM	S TORR/HSUB.COM	HSUB
Temperature **(1)**	Cel	/HSUB.T	S 25/HSUB.T	HSUB
Enthalpy of Vaporization (1)	J/mol	/HVAP	S 90000>HVAP	HVAP
Comment **(2)**	-	/HVAP.COM	S SIEDEPUNKT/HVAP.COM	HVAP
Pressure **(1)**	Torr	/HVAP.P	S 250>HVAP.P	HVAP
Temperature **(1)**	Cel	/HVAP.T	S 20-25/HVAP.T	HVAP
Heat Capacity CP (1)	J/(mol*K)	/CP	S 500-501/CP	CP
Comment **(2)**	-	/CP.COM	S CALORIFICALLY/CP.COM	CP
Temperature **(1)**	F	/CP.T	S CP.T>500	CP
Heat Capacity CpO (1)	J/(mol*K)	/CP0	S 200>CP0	CPO
Comment **(2)**	-	/CP0.COM	S DETERMIN?/CP0.COM	CPO
Temperature **(1)**	Cel	/CP0.T	S 200-220/CP0.T	CPO
Heat Capacity CV (1)	J/(mol*K)	/CV	S 113/CV	CV
Comment **(2)**	-	/CV.COM	S CALCD/CV.COM	CV
Temperature **(1)**	Cel	/CV.T	113/CV.T AND 25/CP	CV
Other Thermochemical Data				
Comment **(2)**	-	/OTHE.COM	S BENZOL/OTHE.COM	OTHE
Description	-	/OTHE.KW	S ENTROPY OF FUSION/OTHE.KW	OTHE

(1) Numeric search field that may be searched using numeric operators or ranges.
(2) Input partly in German.

Transport Phenomena

Search Field Name	Default Units	Fields Searched	Search Examples	Display Codes
Bulk Viscosity (1)	g/cm*s	/BV	S 52-54/BV	BV
Comment **(2)**	-	/BV.COM	S CONCENTRATION/BV.COM	BV
Temperature **(1)**	Cel	/BV.T	S 40-60/BV.T	BV
Dynamic Viscosity (1)	g/cm*s	/DV	S 20/DV.T	DV
Comment **(2)**	-	/DV.COM	S RANGE/DV.COM	DV
Temperature **(1)**	Cel	/DV.T	S 20/DV.T	DV
Kinematic Viscosity (1)	cm**2/s	/KV	S 1.9988-1.9999/KV	KV
Comment **(2)**	-	/KV.COM	S BOILING/KV.COM	KV
Temperature **(1)**	Cel	/KV.T	S 10/KV.T	KV
Self-Diffusion Coefficient (1)	cm**2/s	/SDIF	S SDIF>=25	SDIF
Comment **(2)**	-	/SDIF.COM	S DIAGRAM/SDIF.COM	SDIF
Temperature **(1)**	Cel	/SDIF.T	S 100/SDIF.T	SDIF
Transport Data				
Comment **(2)**	-	/TRAN.COM	S PRESSURE/TRAN.COM	TRAN
Description	-	/TRAN.KW	S THERMAL CONDUCTIVITY/TRAN.KW	TRAN

(1) Numeric search field that may be searched using numeric operators or ranges.
(2) Input partly in German.

Quantum Mechanical Calculations

Search Field Name	Fields Searched	Search Examples	Display Codes
Quantum Mechanical Calculations	/QCC		QCC
Typ	/QCC.TYP	S ANALYSIS/QCC.TYP	QCC
Method	/QCC. MET	S DIRAC/QCC.MET	QCC

DISPLAY and PRINT Formats

Any combination of display fields and formats may be used to display or print answers. Multiple codes must be separated by commas or spaces. The fields are displayed or printed in the order requested. The default format in the ReaxysFile is the dynamic display format QRD (Query Related Data) providing information on identification of Substance (IDE) plus those display fields in which your search terms appear (HIT). Hit-term highlighting is available for the IDE data (AN, CN, COMPAN, COMPC, COMPN, CTYPE, DED, DUPD, FAN, FMF, FS, FW, LSF, MF, RN). Highlighting must be ON during SEARCH in order to use the HIT format.

The ReaxysFile contains more than 120 display field codes. All display codes may be used as valid formats in the DISPLAY and PRINT commands.

DISPLAY OF REACTION DATA

Substance data and reactions are located in different file segments. After searching for a substance or for substance data, three options are available:
1. Show reactions where the substance is the reaction product (RXPRO).
2. Show reactions with the substance acting as a reactant (RXREA).
3. Display all reactions (RX).

After searching for reaction data (/RX.XYZ) use the display code "RX" to show reactions.

Format	Definition	Examples
RXPRO	Reactions with the searched substance as a product	D L4 RXPRO
RXREA	Reactions with the searched substance as a reactant	D RXREA 1-2
RX	Reactions, only available when searched for reaction data	D RX

DISPLAY AND PRINT FORMATS

All predefined formats are listed in a hierarchical order, whereby the indented subformats are included in the previous format.

Format	Content (corresponding DISPLAY FORMAT or FIELD Codes)	Examples
ALL **(1)**	All display fields of CHE, IDE, MCS, PED, PHY, RX, SEP (lengthy display)	DISPLAY ALL
ALLPAT	All patent references for a compound	D ALLPAT
ALLREF	All references for a compound	D ALLREF
CHE **(2)**	Chemical Data (CDER, INP, PUR, RSTR)	D CHE L5 1-4
CDER	Chemical Derivative (CDER)	D CDER
INP	Isolation from Natural Product (INP)	DIS L5 1-5 INP
PUR	Purification (PUR)	DIS L4 PUR
RSTR	Related Structure (RSTR)	D L2 1-3 RSTR
RX **(3)**	Reaction (RX)	DIS RX 1-3
HIT **(4)**	All fields containing HIT terms	D HIT 1-3
IDE **(2)**	Identification of Substance (AUN, BPR, AN, CN, COMPAN, COMPC, COMPN, CTYPE, DED, DUPD, FA, FAN, FMF **5)**, FW, LSF, MF, RN, STR, INCHI, AINCHI, MARKREF)	DISPLAY L1 IDE

DISPLAY AND PRINT FORMATS (cont'd)

Format	Content (corresponding DISPLAY FORMAT or FIELD Codes)	Examples
MCS **(1)**	Multi-Component Systems (ADSM, ASSM, BSPM, EDM, ENEM, LLSM, LSSM, LVS, ODM, MECM, TRAM, SOL)	D 1-6 MCS
ADSM	Adsorption (MCS) (ADSM)	DIS ADSM
ASSM	Association (MCS) (ASSM	DIS ASSM L3 5
BSPM	Boundary Surface Phenomena (MCS) (BSPM)	D L5 BSPM 1-4
EDM	Electrical Data (MCS) (AZE)	DISPLAY EDM
ENEM	Energy Data (MCS) (ENEM)	DIS L5 1 3 5 ENEM
LLSM	Liquid/Liquid System (MCS) (LSSM)	DIS L8 1 2 LSSM
LSSM	Liquid/Solid System (MCS) (LSSM)	
LVS **(2)**	Liquid/Vapour System Data (MCS) (AZE, CPEM, LVSM)	D LVS
AZE	Azeotropes (MCS) (AZE)	DISPLY AZE L8
CPEM	Complex Phase Equilibria (MCS) (CPEM)	DISPLAY CPEM L7 2 5
LVSM	Liquid Vapour System (MCS) (LVSM)	DIS L7 1-5 LVSM
MECM	Mechanical and Physical Property (MCS) (MECM)	D MECM L3
ODM	Optical Data (MCS) (ODM)	DIS ODM L7 3
TRAM	Transport Phenomena (MCS) (TRAM)	D TRAM
SOL **(2)**	Solution Behaviour (MCS) (CMC, HNC, POW, SLB, SLBP, SOLM)	DIS SOL
CMC	Critical Micelle Concentration (MCS) (CMC)	DIS CMC L7 1-10
HNC	Henry Constant (MCS) (HNC)	DIS HNC 1-5
POW	Partition Constant (Octan-1-ol/Water) (MCS) (POW)	Print POW
SLB	Solubility (MCS) (SLB)	DIS L4 1-2 SLB
SLBP	Solubility Product (MCS) (SLBP)	DIS SLBP
SOLM	Solution Behaviour (MCS) (SOLM)	DISPLAY SOLM
PED **(2)**	Pharmacological and Ecological Data (PHARM, ECO, USC)	DISPLAY PED L5
PHARM	Pharmacological Data (PHARM)	DIS L3 PHARM 1-6
ECO **(2)**	Ecological Data (BIO, BIOD, COEV, ECDH, ECDP, ECS, ECTD, ECTOX, EOD, EXCA, USC)	D ECO
BIO	Biological Behaviour (BIO)	D BIO 1-6
BIOD	Biodegration (BIOD)	DIS L40 3 BIOD
COEV	Concentration in Environment (COEV)	DISPLAY COEV L23
ECDH	Abiotic Degradation, Hydrolysis (ECDH)	D ECDH L5 3 6
ECDP	Abiotic Degradation, Photolysis (ECDP)	D ECDP L5 3 6
ECS	Stability in Soil (ECS)	D ECS L9
ECTD	Ecological Mobility: Transport and Distribution (ECTD)	DIS ECTD 10
ECTOX	Ecotoxicology (ECTOX)	DIS ECTOX 1 5
EOD	Oxygen Demand (EOD)	DIS EOD
EXCA	Exposure Assessment (EXCA)	D 1-2 EXCA
USC	Laboratory Use and Handling (USC)	D L3 1-5 USC
PHY **(1)**	Physical Properties (ECB, ELEP, FINFO, MAGP, MECP, OPTP, SAG, SEP, SF, SPE, THE, TRA)	DISPLAY PHY L6 1
ECB **(2)**	Electrochemical Behaviour (DE, ELCB, ELCH, ELYC, IEP, POT, XS)	DIS ECB
DE	Dissociation Exponent (DE)	DIS L8 DE
ECLB	Electrochemical Behaviour Description (ECLB)	D ECLB 5
ELCH	Electrochemical Cell	D ELCH 5
ELYC	Electrolytic Conductivity	D ELYC 5
IEP	Isoelectric Point (IEP)	DIS IEP L9 1-5
POT	Electrochemical Characteristics (POT)	D POT 1 3 7
XS	Cross Section (XS)	DIS L2 XS
ELEP **(2)**	Electrical Properties DIC, DICS, ELE)	DISPLAY ELEP
DIC	Dielectric Constant (DIC)	PRINT DIC L9 1-2
DICS	Static Dielectric Constant (DICS)	DIS L3 1-5 DICS
ELE	Electrical Data (ELE)	DIS ELE L6
MAGP **(2)**	Magnetic Properties (MSUS, MAG)	D L3 MAGP
MSUS	Magnetic Susceptibility (MSUS)	DIS MSUS 1-5
MAG	Magnetic Data (MAG)	DIS MAG L3 1 2
MECP **(2)**	Physical and Mechanical Properties (CMP, DEN, MEC, SOUND, ST)	DIS L9 1-3 MECP
CMP	Compressibility (CMP)	D 1-5 CMP
DEN	Density of the Liquid (DEN)	DIS DEN 1-5

DISPLAY AND PRINT FORMATS (cont'd)

Format	Content (corresponding DISPLAY FORMAT or FIELD Codes)	Examples
MEC	Mechanical Properties (MEC)	D MEC L8
SOUND	Acoustic Properties (SOUND)	DIS SOUND 1-6
ST	Surface Tension (ST)	PRINT L3 ST
TEL	Thermal Expansion	D TEL
OPTP **(2)**	Optical Properties (CDIC, OPT, ORD, ORP, MUT, RI)	D OPTP
CDIC	Circular Dichroism (CDIC)	DISPLAY L1 CDIC
OPT	Optics (OPT)	DIS OPT L
ORD	Optical Rotatory Dispersion (ORD)	D L1 ORD
ORP	Optical Rotatory Power (ORP)	D L3 1-4 ORP
MUT	Mutarotation (MUT)	DIS MUT
RI	Refractive Index (RI)	DISPLAY L7 RI
SAG **(1)**	State of Aggregation (CRY, GAS, LIQ)	DIS SAG L3
CRY	Crystals (CDEN, CPD, CRYPH, CSG, CSYS, CTP, DP, MP, SP, TP)	D L3 1-7 CRY
CDEN	Density of the Crystal (CDEN)	D CDEN 1-3
CPD	Crystal Property Description (CPD)	DIS CPD 1-3
CRYPH	Crystal Phase Description (CRYPH)	PRINT 1-5 CRYPH
CSG	Crystal Space Group (CSG)	DISPLAY CSG
CSYS	Crystal System (CSYS)	D CSYS 1-5
CTP	Crystal Phase Transition Point (CTP)	DIS 1-3 L8 CTP
DP	Decomposition Point (DP)	D 1-5 DP
MP	Melting Point (MP)	DIS MP L3
SP	Sublimation Point (SP)	D SP
TP	Triple Point (TP)	DIS TP 1-5
GAS **(2)**	Gases (CRD, CRP, CRT, CRV, GP, VP)	DIS GAS 1-3
CRD	Critical Density (CRD)	D CRD
CRP	Critical Pressure (CRP)	D CRP L3
CRT	Critical Temperature (CRT)	DISPLAY CRT L8
CRV	Critical Volume (CRV)	DIS CRV L3 1-5
GP	Gas Phase Description (GP)	DISPLAY L5 GP
VP	Vapour Pressure (VP)	D VP 1-6
LIQ **(2)**	Liquids (BP, LIQPH, LPTP)	DIS 1-2 LIQ
BP	Boiling Point (BP)	D L3 BP
LIQPH	Liquid Phase Description (LIQPH)	D LIQPH
LPTP	Transition Point of Liquid Modification (LPTP)	D LPTP 1-10
SEP **(2)**	Structure and Energy Parameter (CIP, CNF, DFM, DM, EBC, EDIS, GEO, IP, POL)	DISPLAY L3 SEP
CIP	Electron Binding (CIP)	DIS CIP 1-3
CNF	Conformation (CNF)	DIS L1 1-2 CNF
DFM	Molecular Deformation (DFM)	DIS DFM
DM	Dipole Moment (DM)	D DM L5
EBC	Energy Barrier of Conformation (EBC)	D L3 EBC
EDIS	Energy of Dissoziation (EDIS)	D L4 1-5 EDIS
GEO	Interatomic Distance and Angle (GEO)	DISPLAY GEO
IP	Ionization Potential (IP)	DIS IP
POL	Electrical Polarizability (POL)	DIS L3 1-3 POL
SF **(2)**	Safety Data (FP)	DISPLAY SF L8
FP	Flash Point (FP)	D FP 1-10
SPE **(1)**	Spectroscopic Data (ESR, FLU, IR, LUM, MS, NMR, NQR, OSM, PHO, RAS, ROT, UVS)	DIS L4 SPE 1-4
ESR	ESR Data (ESR)	D ESR L9
FLU	Fluorescence (FLU)	DISPLAY 1-5 FLU
IR	Infrared Spectrum (IR)	DIS IR 1-10
REACH	REACH relevant data (MP SP BP VP ORP RI MUT DEN DE SLB CP CV HFOR HVAP ECO PHARM FP)	DIS REACH

DISPLAY AND PRINT FORMATS (cont'd)

Format	Content (corresponding DISPLAY FORMAT or FIELD Codes)	Examples
LUM	Luminescence (LUM)	D LUM
MS	Mass Spectrum (MS)	DIS MS 5
NMR	Nuclear Magnetic Resonance (NMR)	DISPLAY NMR L1 1
NQR	Nuclear Quadrupole Resonance (NQR)	DIS NQR
OSM	Other Spectroscopic Methods (OSM)	D L5 OSM
PHO	Phosphorescence (PHO)	DIS PHO 1-4
RAS	Raman Spectrum (RAS)	D L12 1-5 RAS
ROT	Rotational Spectrum (ROT)	DIS ROT
UVS	UV and Visible Spectrum (UVS)	DISPLAY L4 1 UVS
THE **(2)**	Thermodynamic Properties (CP, CPO, CV, HCOM, HFOR, HFUS, HHDG, HPT, HSUB, HVAP, OTHE)	D THE
FINFO	Further Information (FINFO)	DIS L7 1-5 FINFI
CP	Heat Capacity CP (CP)	D L2 CP
CPO	Heat Capacity CPO (CPO)	D CPO
CV	Heat Capacity CV (CV)	DIS L3 CV
HCOM	Enthalpy of Combustion (HCOM)	PRINT L3 HCOM
HFOR	Enthalpy of Formation (HFOR)	D HFOR
HFUS	Enthalpy of Fusion (HFUS)	D HFUS
HHDG	Enthalpy of Hydrogenation (HHDG)	DISPLAY 1-3 HHDG
HPT	Enthalpies of Other Phase Transitions (HPT)	D L8 HPT
HSUB	Enthalpy of Sublimation (HSUB)	PRINT L3 HSUB
HVAP	Enthalpy of Vaporization (HVAP)	D HVAP
OTHE	Other Thermodynamic Data (OTHE)	D OTHE
TRA **(2)**	Transport Phenomena (BV, DV, KV, SDIF, TRAN)	D TRA 2, 5
BV	Bulk Viscosity (BV)	D L2 BV
DV	Dynamic Viscosity (DV)	D DV L3 1-35
KV	Kinematic Viscosity (KV)	D KV 17
SDIF	Self-diffusion Coefficient (SDIF)	D SDIF L17
TRAN	Transport Data (TRAN)	D L1 TRAN 1-10
QRD **(4)**	Query Related Data (default: dynamic format IDE, HIT)	D 5 QRD
FA	Field Availability	D FA 1-5

(1) Please note, that this format may contain data from multiple fee units.
(2) All separate custom display fields of this predefined format are together charged as one fee unit.
(3) Use RX to display reactions when searched for reaction data (/RX.XYZ). Use RXPRE, RXREA or RX. (see preceding table) to display reactions after searching for a substance.
(4) Default: Dynamic display format QRD (Query Related Data) providing information on Identification of Substance (IDE) plus those display fields in which your search terms appear (HIT)
(5) For compounds consisting of one fragment, FMF is identical with MF and only MF is displayed.

SELECT, ANALYZE, and SORT Fields

The SELECT command is used to create E-numbers containing terms taken from the specified field in an answer set.

The ANALYZE command is used to create an L-number containing terms taken from the specified field in an answer set.

The SORT command is used to rearrange the search results in either alphabetic or numeric order of the specified field(s).

SELECT, ANALYZE, and SORT Fields (cont'd)

Field Name	Field Code	ANALYZE/ SELECT (1)	SORT
Abiotic Degradation, Hydrolysis; Degradation Product AN	ECDH.AN	Y **(2)**	N
Abiotic Degradation, Photolysis; Degradation Product AN	ECDP.AN	Y **(2)**	N
Accession Number	AN	Y	N
Adsorption (MCS), Partner AN	ADSM.PAAN	Y **(2)**	N
Association (MCS), Partner AN	ASSM.PAAN	Y **(2)**	N
Azeotropes AN	AZE.PAAN	Y **(2)**	N
Basic Preferred Registry Number	BPR	Y	N
Biodegradation, Degradation Product AN	BIOD.AN	Y **(2)**	N
Boundary Surface Phenomena (MCS), Partner AN	BSPM.PAAN	Y **(2)**	N
CAS Registry Number	RN	Y	N
Chemical Derivative AN	CDER.AN	Y **(2)**	N
Chemical Name	CN	Y	N
Complex Phase Equilibria Partner AN	CPEM.PAAN	Y **(2)**	N
Composition: Compound AN	COMPAN	Y	N
Ecotoxicology, Metabolite AN	ECTOX.AN	Y **(2)**	N
Electrical Data, Partner AN	EDM.PAAN	Y **(2)**	N
Electrochemical Characteristics, Product AN	POT.PAN	Y **(2)**	N
Energy Data (MCS), Partner AN	ENEM.PAAN	Y **(2)**	N
Enthalpy of Hydrogenation Product AN	HHDG.AN	Y **(2)**	N
Fragment AN	FAN	Y	N
Fragment Molecular Formula	FMF	Y	N
Linearized Structure Formula	LSF	Y	N
Liquid/Liquid System, Partner AN	LLSM.PAAN	Y	N
Liquid/Solid System, Partner AN	LSSM.PAAN	Y **(2)**	N
Liquid/Vapour System, Partner AN	LVSM.PAAN	Y **(2)**	N
Mechanical and Physical Property (MCS), Partner AN	MECM.PAAN	Y **(2)**	N
Molecular Formula	MF	Y (default)	N
Molecular Weight	MW (FW)	Y	N
Optical Data (MCS), Partner AN	ODM.PAAN	Y	N
Other Source	XREF.SO	Y	N
Patent Number	PN	Y **(2)**	N
Pharmacological Data, Metabolite AN	PHARM.AN	Y	N
Product AN	RX.PAN	Y	N
Reactant AN	RX.RAN	Y	N
Related Structure Referenced AN	RSTR.PAAN	Y	N
Solution Behaviour, Partner AN	SOLM.PAAN	Y	N
Stage Reactant AN	RX.SRAN	Y	N
Transport Phenomena (MCS), Partner AN	TRAM.PAAN	Y	N

(1) HIT may be used to restrict terms extracted to terms that match the search expression used to create the answer set,e.g., SEL HIT RN.

(2) SELECT HIT and ANALYZE HIT are not valid with this field.

STRUCTURE SEARCHING

Structure Search Terms

Terms (1)	Search Examples
L-numbers of structures built using the STRUCTURE command or uploaded from STN Express (Boolean logic allowed between the L-numbers)	SEARCH L1 FAM SAM SEA L1 AND L2 SSS FUL
L-numbers of screen sets created using the SCREEN command (Boolean logic allowed between the L-numbers)	S L3 OR L4 SSS SAM
L-number of a structure built using the STRUCTURE command or uploaded from STN Express combined with L-numbers of screen sets created using the SCREEN command (Boolean logic allowed between the L-numbers)	S L1 AND L2 NOT L3

(1) The L-number answer set from a structure search may be combined with dictionary or factual terms, e.g. 'S L6 AND AMINO' or 'S L3 AND IR?/FA'.

Types of Structure Searching

Type	Definition	Search Code	Search Examples
Substructure (default)	Search for substances which match the query. Substitution is allowed at all open positions. Additional components may be retrieved	SSS	SEARCH L1 SSS FUL S L2 OR L3 SSS SAM S L7 SSS RAN
Closed Substructure	Search for substances which match the query exactly. Substitution is allowed at positions opened by CONNECT. Additional components may be retrieved.	CSS	SEARCH L1 CSS FUL S L2 OR L3 CSS S L4 NOT L5 CSS RAN
Family	Search for substances which match the query exactly. Additional components may be retrieved.	FAM	S L6 FAM SAM
Exact	Search for substances which match the query exactly.	EXA	SEA L5 EXA FUL

Scopes of Structure Searches

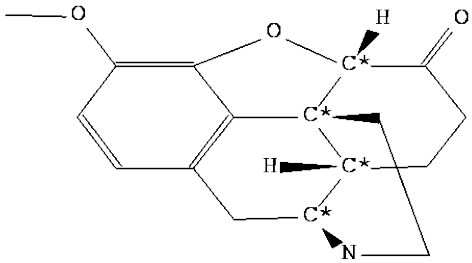
Type	Definition	Search Code	Search Examples
Sample (default)	Search a fixed 5% of the file	SAM	SEARCH L3 EXA SAM S L6 NOT L7 SSS SAM
Full	Search 100% of the file.	FUL	S L5 OR L8 SSS FUL
Range	Search a user-specified portion of the file.	RAN	S L4 RAN=(5471081,) S L3 FAM RAN=(77542, 80001)
Subset Sample	Search a fixed sample of an answer set created by a search in ReaxysFile.	SUB SAM	S L7 CSS SUB=L5 SAM
Subset Range	Search a user-specified portion of an answer set created by a search in ReaxysFile.	SUB RAN	S L3 SUB=L2 RAN=(,72810)
Subset Full	Search 100% of an answer set created by a search in ReaxysFile.	SUB FUL	S L8 SUB=L6 FAM FUL

SAMPLE Records

DISPLAY IDE (Substance Identification)

a) Organic Substance

Accession Number (AN):	42574
CAS Reg. No. (RN):	5083-62-5, 74007-29-7, 88269-01-6
Chemical Name (CN):	Nordihydrocodeinon, norhydrocodone, 4,5α-epoxy-3-methoxy-morphinan-6-one, 4,5α-Epoxy-3-methoxy-morphinan-6-on, 4,5α-Epoxy-3-methoxymorphinan-6-one, Dihydro-norcodeinon,hydronorcodeinone
Lin. Struct. Formula (LSF):	C17H19NO3
Molec. Formula (MF):	C17 H19 N O3
Formula Weight (FW):	285.343
InChi Key: (INCHI):	JGORUXKMRLIJSV-YNHQPCIGSA-N
Alternate InChi Key: (AINCHI):	JGORUXKMRLIJSV-YNHQPCIGBC
Compound Type (CTYPE):	heterocyclic
Markush Ref. Count (MARKREF):	0
Entry Date (DED):	1988/06/27
Update Date (DUPD):	2011/01/24



Field Availability:

Code	Name	Occurrence
AN	Accession Number	1
RN	CAS Registry Number	3
CN	Chemical Name	7
LSF	Linearized Structure Formula	1
MF	Molecular Formula	1
FW	Formula Weight	1
INCHI	InChi Key	1
AINCHI	Alternate InChi Key	1
CTYPE	Compound Type	1
MARKREF	Markush Reference Count	1
DED	Entry Date	1
DUPD	Update Date	1
CPD	Crystal Property Description	1
IR	Infrared Spectrum	3
LB	Substance Label	4
MP	Melting Point	4
MS	Mass Spectrum	2
NMR	Nuclear Magnetic Resonance	3
ORP	Optical Rotatory Power	4

PHARM	Pharmacological Data	3

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	31
RX.RAN	Reactant AN	24
RX.PAN	Product AN	7

b) Inorganic Substance (Alloy)

Accession Number (AN):	13766819
Chemical Name (CN):	cerium-nickel, nickel cerium
Lin. Struct. Formula (LSF):	CeNi
Molec. Formula (MF):	Ce Ni
Formula Weight (FW):	198.81
InChi Key: (INCHI):	WITQLILIVJASEQ-UHFFFAOYSA-N
Alternate InChi Key: (AINCHI):	WITQLILIVJASEQ-UHFFFAOYAA
Compound Type (CTYPE):	Alloy
Markush Ref. Count (MARKREF):	0
Entry Date (DED):	2008/06/22
Update Date (DUPD):	2011/01/10

No structure diagram available for this Document

Field Availability:

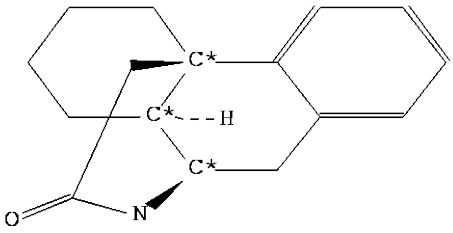
Code	Name	Occurrence
AN	Accession Number	1
CN	Chemical Name	2
LSF	Linearized Structure Formula	1
MF	Molecular Formula	1
FW	Formula Weight	1
INCHI	InChi Key	1
AINCHI	Alternate InChi Key	1
CTYPE	Compound Type	1
MARKREF	Markush Reference Count	1
DED	Entry Date	1
DUPD	Update Date	1
CDEN	Density (Crystal)	2
CP	Heat Capacity Cp	2
CRYPH	Crystal Phase	5
CSG	Crystal Space Group	8
CSYS	Crystal System	1
CTP	Crystal Transition Point	1
ELE	Electrical Data (MCS)	4
ESR	ESR Data	1
HFOR	Enthalpy of Formation	1
LUM	Luminescence	1
MAG	Magnetic Data	12
MEC	Mechanical Property	2
MP	Melting Point	2
MSUS	Magnetic Susceptibility	3
OPT	Optics	1
OSM	Other Spectroscopic Methods	2
PSD	Patent Specific Data	1
QCC	Quantum Chemical Calculations	8
TEC	Thermal Expansion	9
USC	Use of Compound	2

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	8
RX.RAN	Reactant AN	7
RX.PAN	Product AN	1

DISPLAY QRD (Query Related Display, structure query combined with search for spectroscopic data)

Accession Number (AN):	16976
Basic Pref. RN (BPR):	98883-08-0
CAS Reg. No. (RN):	98883-08-0
Chemical Name (CN):	rac-14α-morphinan-16-one, rac-14α-Morphinan-16-on
Lin. Struct. Formula (LSF):	C16H19NO
Molec. Formula (MF):	C16 H19 N O
Formula Weight (FW):	241.333
Compound Type (CTYPE):	heterocyclic
InChi Key: (INCHI):	CUUYMJMGAWRNDJ-OFQRWUPVSA-N
Alternate InChi Key: (AINCHI):	CUUYMJMGAWRNDJ-ZXKMXMATDD
Markush Ref. Count (MARKREF):	0
Entry Date (DED):	1988/06/27
Update Date (DUPD):	2008/05/24



Field Availability:

Code	Name	Occurrence
AN	Accession Number	1
BPR	Basic Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	2
LSF	Linearized Structure Formula	1
MF	Molecular Formula	1
FW	Formula Weight	1
INCHI	InChi Key	1
AINCHI	Alternate InChi Key	1
CTYPE	Compound Type	1
MARKREF	Markush Reference Count	1
DED	Entry Date	1
DUPD	Update Date	1

IR	Infrared Spectrum	1
MP	Melting Point	2
RSTR	Related Structure	1
UVS	UV and Visible Spectrum	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	16
RX.RAN	Reactant AN	13
RX.PAN	Product AN	3

Infrared Spectrum:

Description (.KW)	Solvent (.SOL)	Ref.	Note
Spectrum	CHCl3	1	1

Reference(s):
1. Gates et al., Journal of the American Chemical Society, CODEN: JACSAT, 72, <1950>, 1141,1142

Notes(s):
1. 4000 - 952 cm**(-1)

UV and Visible Spectrum:

Description (.KW)	Solvent (.SOL)	Ref.	Note
Spectrum	methanol	1	1

Reference(s):
1. Gates et al., Journal of the American Chemical Society, CODEN: JACSAT, 72, <1950>, 1141,1142

Notes(s):
1. 230 - 300 nm

DISPLAY RX (Reactions, structure search combined with search for Diels-Alder reactions)

Reaction:
RX

Reaction ID:	11166712
Reactant AN (.RAN):	106909, 11169556
Reactant (.RCT):	maleic anhydride,<<2-(2,2-dibutyl-2-stannahexyl)phenyl>methylthio>benzene
Product AN (.PAN):	84508
Product (.PRO):	cis-1,2,3,4-tetrahydro-2,3-naphthalenedicarboxylic anhydride
React. Struct. Keywords (.SKW):	nonmapped reaction
Record type (.RTYP):	full reaction, has preparation
Number of Bond Changes (.NBC):	3
No. of React. Details (.NVAR):	1
Preparation reactants (.BLB):	106909, 11169556, 84508
Det. React. reactants (.BLC):	106909, 11169556, 84508
No. of References (.NUMREF):	1

```
Reaction Details:
RX
     Reaction RID (.RID):            11166712.1
     Reaction Classification (.CL):  Preparation
     Yield (.YDT):                   89 percent
     Reagent (.RGT):                 lithium perchlorate, acetic acid
     Solvent (.SOL):                 nitromethane
     Other Conditions (.COND):       Electrochemical reaction
     Reaction Type (.TYP):           Diels-Alder reaction
     Product AN (.PRAN):             84508
     Reactant AN (.RCAN):            3596973, 506007
     Solvent AN (.SOLAN):            1698205
     Number of R. steps (.STP):      1
     Yield numerical (.YDN):         89
     Product (.YPRO):                cis-1,2,3,4-tetrahydro-2,3-
                                     naphthalenedicarboxylic anhydride
     Reference(s):
     1. Jinno, Madoka; Kitano, Yoshikazu; Tada, Masahiro; Chiba, Kazuhiro,
        Organic Letters, CODEN: ORLEF7, 1(3), <1999>, 435 - 437
```

DISPLAY ALLPAT (All patents; it is recommended to `SET LINE 100`**)**

```
   ANSWER 1 OF 1 REAXYSFILE COPYRIGHT 2012 Elsevier Properties SA. on STN

     All Patents:
     ALLPAT


Reference:       Patent
Title:           PROCESS FOR PRODUCING UNSATURATED HYDROCARBON COMPOUND
Patent Number:   EP1852408
Inventor:        YOKOTA, Kiyohiko; FUJIKAWA, Shinjiro; OKAMOTO, Takuji
Patent Assignee: IDEMITSU KOSAN CO., LTD.
Abstract:        Disclosed is a method for producing an unsaturated hydrocarbon
                 compound wherein an α-olefin is dimerized by using a catalyst
                 system composed of a  metallocene compound (A) and an oxygen-
                 containing organometallic compound modified with a halogen-
                 containing compound (B). By this method, an unsaturated
                 hydrocarbon compound having unsaturated double bonds in a high
                 ratio, in particular the one having a terminal vinylidene group
                 can be produced
                    efficiently.
Main IPC:        C07C 2/30
Secondary IPC:   C07B 61/00; C07C 11/02; C07C 2/34
                 Priority Number     Priority Date
                 JP2005-44853        2005/02/21
PATENT INFORMATION

Patent Title:    PROCESS FOR PRODUCING UNSATURATED HYDROCARBON COMPOUND
Patent Number     Kind Code  Publ. Date    Application No    Filing Date
Indexed Patent
WO2006/88038      A1         2006/08/24    WO2006-JP302606   2006/02/15    ---
JP2006/232672     A          2006/09/07    JP2005-44853      2005/02/21    ---
EP1852408         A1         2007/11/07    EP2006-713747     2006/02/15    yes
US2009/30255      A1         2009/01/29    US2007-815975     2007/08/10    ---
```

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Internet: www.jaici.or.jp